

Wilson chains are not thermal reservoirs

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Abstract. Wilson chains, based on a logarithmic discretization of a continuous spectrum, are widely used to model an electronic (or bosonic) bath for Kondo spins and other quantum impurities within the numerical renormalization group method and other numerical approaches. In this short note we point out that Wilson chains can *not* serve as thermal reservoirs as their temperature changes by a number of order ΔE when a finite amount of energy ΔE is added. This proves that for a large class of non-equilibrium problems they cannot be used to predict the long-time behavior.

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In 1975 Wilson pioneered [1] the “numerical renormalization group” (NRG) approach to solve the Kondo model. This approach is able to provide numerically exact solutions to the Kondo problem, probably the most important and most influential quantum impurity model. The NRG is by now widely used for a large range of fermionic and bosonic quantum impurity problems both at zero and finite temperature [2].

A quantum impurity problem is defined by some local degree of freedom coupled to a (most often non-interacting) bath. In the case of the classical Kondo model this bath is given by an infinite system of electrons with a constant density of states at the Fermi energy.

Wilson’s numerical solution consists of two main steps. First the bath is discretized using energies defined on a logarithmic grid.

$$\epsilon_{\pm|n|} = \pm \frac{D}{A^{|n|}} \quad (1)$$

This logarithmic grid is optimized for the logarithmic renormalization group flow characteristic for the Kondo model and allows to capture even the exponentially small energy scales characteristic for the Kondo problem. In praxis [2] it is implemented via the so-called Wilson chain, a chain of local sites coupled by nearest neighbor hopping rates which decay exponentially in the distance from the quantum impurity. The second step, the actual renormalization group transformation, strongly builds on this logarithmic discretization [2] but it plays no role for the following discussion.

An exciting recent development is that it is now possible to study quantum impurity problems numerically in non-equilibrium using NRG [3,4,5,6,7]. Especially F. B. Anders and A. Schiller pioneered powerful methods to study quantum quenches [4] and to investigate steady-state transport using many-particle scattering states [5].

Also other numerical methods, most notably time-dependent density matrix renormalization group have been applied to Wilson chains [8].

NRG and the use of Wilson chains has been extremely successful [2]. Therefore it is a relevant question to understand whether there are limitations to this approach. In this short note we briefly discuss a very severe limitation: Wilson chains can not be used as thermal reservoirs. We argue that this implies that for certain classes of non-equilibrium problems Wilson chains give wrong results.

A reservoir is by definition an infinite system which can be used to fix the chemical potential and the temperature. More precisely, when adding a finite amount of particles or a finite amount of energy, the chemical potential and the temperature do not change. While in experimental systems reservoirs are never really infinite, in praxis the large number of electrons, for example in a metallic contact attached to a quantum dot, provides an almost ideal realization of a reservoir.

Within this definition, the Wilson chain can serve as a reservoir for particles as one can check by calculating $\frac{dN}{d\mu}$, for the non-interacting Wilson chain in the absence of the quantum impurity

$$\begin{aligned} \left. \frac{dN}{d\mu} \right|_{\mu=0} &= -2 \sum_{|n| < N_{\text{sites}}} f'(\epsilon_n) \approx \sum_{|\epsilon_n| < T, |n| < N_{\text{sites}}} \frac{1}{2T} \\ &\approx \frac{N_{\text{sites}}}{T} \rightarrow \infty. \end{aligned} \quad (2)$$

Here N is the total number of particles, $f(\epsilon) = 1/(e^{(\epsilon-\mu)/T} + 1)$ is the Fermi function and the factor 2 accounts for the spin degeneracy. $\frac{dN}{d\mu}$ diverges with the number of sites in the Wilson chain implying that in practical calculations the chemical potential stays constant when, for example, N increases by 1.

In contrast, the total energy of the Wilson chain and its derivative with respect to temperature T remain finite in the limit $N_{\text{sites}} \rightarrow \infty$ for finite discretization parameter $\Lambda > 1$.

$$\frac{dE}{dT} = -2 \sum_n \frac{\epsilon_n^2}{T} f'(\epsilon_n) \approx 4 \int_{-\infty}^{\infty} dn \frac{\Lambda^{-2n} e^{\Lambda^{-n}}}{(1 + e^{\Lambda^{-n}})^2} = \frac{4 \ln 2}{\ln \Lambda} \quad (3)$$

In practical calculations Λ is never very close to 1 (an often used value is $\Lambda = 2$) therefore dE/dT is a number of order 1!

This has severe practical implications for non-equilibrium situations. Consider, for example, a quantum quench where at time $t = 0$ suddenly a hybridization of strength Γ is switched on, which couples an Anderson impurity to a Wilson chain at $T = 0$. The following time evolution conserves energy. The ground state energy of the system with finite hybridization is approximately lower by Γ than the energy of the initial state. Assuming that the system equilibrates, Eq. (3) implies that final state has a huge temperature of order $\Gamma \ln \Lambda$, much larger than the Kondo temperature. In contrast, an Anderson impurity coupled to a real reservoir, where dE/dT diverges with system size, relaxes to the $T = 0$ groundstate in the thermodynamic limit. While in real systems the energy can be transported away from the quantum impurity to infinity this is not possible for the Wilson chain due to its finite heat capacity. Our argument proves that in the long time limit a wrong result is obtained for all quantum quenches where the energy of the initial configuration is higher than the ground state energy by an amount of the order of the energy scale one is interested in. With Eqn. (3) one can estimate quantitatively the heating of the quantum impurity. This can serve as a quantitative estimate of the backreaction to the quantum impurity which arises as the Wilson chain is not able to transport energy away to infinity.

It is less clear to what extent the short-time dynamics is affected but even in this case it would not be surprising if the problem to transport energy away is of relevance even shortly after a quantum quench. Recently, P. Schmitteckert [9] made a closely related observation by studying the time-evolution of a wave packet on a Wilson chain: the wave packet piles up in a “Wilson Tsunami” and is not able to reach the end of the chain.

It is an interesting question whether and to what extent the finite heat capacity of Wilson chains is also of importance when using scattering states to treat steady-state non-equilibrium [5]. Consider, for example, a quantum dot in the Kondo regime in the presence of a finite bias voltage [10]. In this case the finite product of voltage and current implies that power is pumped into the system. This power is ultimately dissipated in infinite reservoirs where the precise form of the dissipation mechanism is usually not important as the relaxation occurs far away from the impurity. In the case of an infinite Wilson chain where energy cannot be added without modifying the bath, one can suspect that (as in the case of a quantum quench) the interacting non-equilibrium situation cannot be treated properly. Interestingly, present NRG implementations seem not to be

able to recover the result [11,10] that the Kondo peak in the spectral function splits in the presence of a bias voltage which exceeds the Kondo temperature. This result is well established by (renormalized) perturbation theory and controlled one-loop renormalization group [10] calculations. Possibly, the numerical results which have been obtained for the Anderson model where not sufficiently deep in the Kondo regime to see the splitting. Alternatively, it is also possible that the use of Wilson chains is the origin of the problem. Note, however, that also other numerical approaches which are not relying on Wilson chains have presently problems to obtain the splitting [12].

In contrast to the fermionic Wilson chain, for bosons the heat capacity of the Wilson chain is infinitely large due to the possibility to put a large number of bosons into the states with very low energy (replacing the plus by a minus sign in the integral of Eq. (3) leads to a divergence). In practical NRG implementations [2], however, only a finite number of bosons is taken into account which renders dE/dT again finite.

In conclusion, it seems that the use of Wilson chains for non-equilibrium problems is a much more dangerous approximation compared to the equilibrium case as Wilson chains cannot take up finite amounts of energy without changing their properties.

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References

1. K. G. Wilson, Rev. Mod. Phys. **47**, (1975) 773.
2. R. Bulla, T.A. Costi, and T. Pruschke, Rev. Mod. Phys. **80**, (2008) 395.
3. T. A. Costi, Phys. Rev. B **55**, (1997) 3003.
4. F. B. Anders and A. Schiller, Phys. Rev. Lett. **95**, (2005) 196801; F. B. Anders and A. Schiller, Phys. Rev. B **74**, (2006) 245113.
5. F. B. Anders, Phys. Rev. Lett. **101**, 066804 (2008).
6. D. Roosen, M. R. Wegewijs, W. Hofstetter, Phys. Rev. Lett. **100**, 087201 (2008); A. Hackl, D. Roosen, S. Kehrein, and W. Hofstetter, Phys. Rev. Lett. **102**, (2009) 196601.
7. S. Schmitt and F. B. Anders, Phys. Rev. Lett. **107**, (2011) 056801.
8. L. G. G. V. Dias da Silva¹, F. Heidrich-Meisner, A. E. Feiguin, C. A. Büsser, G. B. Martins, E. V. Anda, E. Dagotto, Phys. Rev. B **78**, (2008) 195317.
9. P. Schmitteckert, J. Phys.: Conf. Ser. **220**, (2010) 012022.
10. A. Rosch, J. Kroha, and P. Wölfle, Phys. Rev. Lett. **87**, (2001) 156802; A. Rosch, J. Paaske, J. Kroha, and P. Wölfle, Phys. Rev. Lett. **90**, (2003) 076804 ; A. Rosch, J. Paaske, J. Kroha, P. Wölfle, J. Phys. Soc. Jpn. **74**, 118 (2005). N. Shah and A. Rosch, Phys. Rev. B **73**, (2006) 081309R.
11. Y. Meir, N. S. Wingreen, P. A. Lee Phys. Rev. Lett. **70**, (1993) 2601.
12. L. Mühlbacher, D. F. Urban, and A. Komnik, Phys. Rev. B **83**, (2011) 075107.